V International Conference on Computational Methods for Coupled Problems in Science and Engineering
COUPLED PROBLEMS 2013
S. Idelsohn, M. Papadrakakis and B. Schrefler (Eds)

COUPLING LEVEL SET METHODS WITH BOUNDARY INTEGRAL METHODS FOR FREE SURFACE POTENTIAL FLOWS

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Key words: Potential flows, Level Set methods, Boundary Integral Methods, Wave Breaking, Drop formation

Abstract. Non viscid and rotational free fluid flows in moving domains can be used to model various physical phenomenons such us wave breaking, droplet and bubble break up dynamics and electrostatically charged drop distortion, among others.

The classical lagrangian fully non linear potential flow model can be recasted in a complete Eulerian formulation using the Level Set approach. The coupled system of partial differential equations is approximated using a Boundary Integral method, to calculate the moving front velocity, and the Level Set method to update the position of the front. The numerical methods involved are: a linear Boundary Element method for the laplacian equation and first order upwind schemes for the Level Set hyperbolic equations. This novel approach has turn out to be very robust and versatile, due to the capability of the Level Set method to handle topological changes of the moving domain.

Full details of how to arrive to the Eulerian formulation of the model equations will be presented and the numerical schemes of the coupled system will be also described. Several computational results will be addressed: The propagation and shoaling of a solitary wave over a sloping beach and the collapse of an infinite fluid column under the action of surface tension forces. Recent results on the evolution and distortion of charged droplets and subsequent Coulombic fission will be presented in more detail

1 INTRODUCTION

In this paper we present a class of problems in the field of fluid mechanics that can be modeled using the potential flow assumptions, that is, inviscid and incompressible fluids moving under an irrotational velocity field. While these are significant assumptions, in the presence of moving boundaries, the resulting equations is a non linear partial differential equation, which adds considerable complexity to the computational problem. In the literature this model is often called the fully non linear potential flow model (FNPFM). Several interesting and rather complicated phenomenon are described using the FNPFM, as for example, Helle-Shaw flows, jet evolution and drop formation, sprays and electrosprays, wave propagation and breaking mechanisms, etc, see [1], [2], [3].

Level Set Methods (LSM) [4] are widely used in fluid mechanics, as well as other fields such as medical imaging, semiconductor manufacturing, ink jet printing, and seismology. The LSM is a powerful mathematical tool to move interfaces, once the velocity is known. In many physical problems, the interface velocity is obtained by solving the partial differential equations system used to model the fluid/fluids flow. The LSM is based on embedding the moving front as the zero level set of one higher dimensional function. By doing so, the problem can be formulated in a complete Eulerian description and topological changes of the free surface are automatically included. The equation for the motion of the level set function is an initial value hyperbolic partial differential equation, which can be easily approximated using upwind finite differences schemes.

Recently, the LSM has been extended to formulate problems involving the transport and diffusion of material quantities, see [5]. In [5] model equations and algorithms are presented together with the corresponding test examples and convergence studies. This led to the realization that the nonlinear boundary conditions in potential flow problems could also be embedded using level set based methods. As a result, the FNPFM can also be formulated with an Eulerian description with the associated computational advantages. Several difficult problems that have been already approximated using this novel algorithm are wave breaking over sloping beaches [7], [8]; the Rayleigh Taylor instability of a water jet [9]; a two inviscid fluid system of different densities [10]; and the evolution of charged and uncharged droplets under the action of an electrical field [12].

2 POTENTIAL FLOW EQUATIONS

In this section we first we present the general conservations laws applied to a fluid volume V and then, by introducing the required assumptions, we derive the potential flow model equations. Denote by $\rho = \varrho(P, t)$ the volumetric mass density of the continuous medium at point P and at time t and $\mathbf{u}$ the velocity field, the mass conservation law is

$$\mathrm{D}_t\rho + \rho \,\mathrm{div}\, \mathbf{u} = 0. \tag{1}$$

For the conservation of momentum, Newton's law is applied to a fluid volume V:

$$\mathrm{D}_t \int_V \mathbf{u}\, \rho \mathrm{d}V = \int_V \mathbf{g}\, \rho \mathrm{d}V + \int_{\partial V} \tau(\mathrm{d}\mathbf{s}). \tag{2}$$

The term in left hand side of this equation is the rate of change with time of the momentum associated with volume V when dragged by the continuous medium. The first term in the right hand side corresponds to the volumetric forces inside V, generated by a vector field per unit mass $\mathbf{g}$, usually the gravitational field. The second term represents the "contact" forces applied by the rest of the medium over the part in V. The Cauchy's tensor τ is a linear operator field that is obtained from specific relationships which depend on the material, the so called constitutive relations. We are interested in inviscid fluids which verify the Pascal's law: $\tau(\mathrm{d}\mathbf{s}) = -p\mathrm{d}\mathbf{s}$, where p is the pressure scalar field. Green's formula,

$$\int_{\partial V} -p \, \mathrm{d}\mathbf{s} = \int_V -\nabla p \, \mathrm{d}V,$$

shows that contact forces may be computed as a kind of volume forces with density $-\nabla p$. For a small volume δV dragged by the fluid, equation (2) can be written:

$$\mathrm{D}_t(\mathbf{u}\,\rho\delta V) = (\mathbf{g}\,\rho - \nabla p)\delta V. \tag{3}$$

Due to the mass conservation law, $\mathrm{D}_t(\rho\delta V) = 0$, equation (3) leads to the Euler equation:

$$\mathrm{D}_t\mathbf{u} = \partial_t\mathbf{u} + \partial_{\mathbf{u}}\mathbf{u} = \mathbf{g} - \frac{1}{\rho}\nabla p. \tag{4}$$

If $\mathbf{g}$ is a uniform field it comes from the gradient of a potential function:

$$\mathbf{g} = -\nabla U(P), \;\; U(P) = -\mathbf{g}\cdot(P - O),$$

where $P - O$ is the position vector of the point P.

Now we introduce the potential flow restrictions. Assuming constant fluid density and an irrotational flow regime, curl $\mathbf{u} = 0$, there exists an scalar field ϕ such that $\mathbf{u} = \nabla\phi$ and Eqn.(1) becomes

$$\Delta\phi = 0. \tag{5}$$

Outside of the fluid domain, and separated by a free boundary, there is a gas at pressure p_a that, for now, is assumed to be constant.

Using the vectorial relationship $\nabla\mathbf{u}^2/2 = \partial_{\mathbf{u}}\mathbf{u} + \mathbf{u} \times (\mathrm{curl}\ \mathbf{u})$, $\mathbf{u} = \nabla\phi$ and div $\mathbf{u} = 0$ we have

$$\nabla\left(\partial_t\phi + \frac{1}{2}\mathbf{u}^2 + \frac{p}{\rho} + U\right) = 0.$$

Performing the first integration,

$$\partial_t\phi + \frac{1}{2}\mathbf{u}^2 + \frac{p}{\rho} + U = C(t),$$

where $C(t)$ is an arbitrary function of time, which can be chosen in such a way that the previous relation can be written:

$$\partial_t\phi + \frac{1}{2}\mathbf{u}^2 + \frac{p - p_a}{\rho} + U = 0.$$

Now using the obvious relation $\partial_t\phi + \mathbf{u}^2 = \partial_t\phi + \partial_{\mathbf{u}}\phi = \mathrm{D}_t\phi$, we finally obtain

$$\mathrm{D}_t\phi - \frac{1}{2}\mathbf{u}^2 + \frac{p - p_a}{\rho} + U = 0. \tag{6}$$

Now, let Ω_t be a closed 3D moving fluid domain, Γ_t the free surface bounday at time t and Q the position vector of a fluid particle on the front (Q will be precisely defined in the next section). To close the system we have to add the conditions at the moving boundary:

- The kinematic boundary condition, which states that the particles in the free front move with velocity $\mathbf{u}$, $D_tQ = \mathbf{u}$.
- The Dynamic boundary condition, which comes from the conservation of momentum when we impose the continuity of the stress tensor across the free boundary,

  $$D_t\phi = f,$$

  being

  $$f = -U + \frac{1}{2}\mathbf{u}^2 - (\frac{p - p_a}{\rho}).$$

Therefore, the Lagrange formulation of the potential flow equations is:

$$\begin{aligned} \mathbf{u} &= \nabla\phi \text{ in } \Omega_t && (7)\\ \Delta\phi &= 0 \text{ in } \Omega_t && (8)\\ D_tQ &= \mathbf{u} \text{ on } \Gamma_t && (9)\\ D_t\phi &= f \text{ on } \Gamma_t && (10) \end{aligned}$$

Outside the fluid domain we may consider several possible scenarios, as for example:

1. An infinite exterior fluid at rest.
2. An infinite exterior moving fluid of different density (an inviscid two fluid system).
3. A dielectric gas under the action of a uniform electric field at the far field.

For each of these scenarios the corresponding model equations in the exterior domain have to be coupled with system (7)-(10), and a rich variety of dynamics arises depending upon the expression of $f|_{\Gamma_t}$ in each particular case.

Next, the boundary conditions posed on the moving front are going to be embeded in higher dimension equations using the level set techniques. This procedure will lead to the complete Eulerian formulation of the potential flow equations.

3 THE LEVEL SET METHOD

The Level Set method is a mathematical tool very adequate to follow interfaces which move with a given velocity field. The key idea is to view the moving front as the zero level set of one higher dimensional function called the level set function. One main advantage of this approach comes when the moving boundary changes topology, and thus a simple connected domain splits into separated disconnected domains.

Let be Γ_t the set of points lying in the surface boundary at time t. This surface is defined through the zero level set of the scalar field $\Psi = \psi(P, t)$:

$$\Gamma_t = \{Q|\psi(Q, t) = 0\}. \tag{11}$$

To identify the fluid particles, the configuration at t_0 (reference configuration) is used:

$$\Gamma_{t_0} = \{Q_0|\psi(Q_0, t_0) = 0\}. \tag{12}$$

The particle movement is specified through the function

$$Q = R(Q_0, t), \tag{13}$$

which gives the position $Q \in \Gamma_t$ of the fluid particle $Q_0 \in \Gamma_{t_0}$. The particle Q_0 velocity is calculated using the convective derivative D_t ("following the particle"):

$$\mathbf{u} = D_t Q = \frac{\mathrm{d}}{\mathrm{d}\epsilon} R(Q_0, t + \epsilon)\bigg|_{\epsilon=0}. \tag{14}$$

According to definition (11), we have $\psi(R(Q_0, t), t) = 0$. Deriving with respect to time and applying the chain rule, we obtain

$$\partial_t \Psi + \mathbf{u} \cdot \nabla \Psi = 0, \tag{15}$$

which has to be completed with the value of the level set function at time $t = 0$, usually set to be the signed distance function to the initial front,

$$\Psi(P, 0) = s(P)d(P),$$

being $d(P)$ the distance from the point P to the surface at the initial configuration Γ_0, $s(P) = -1$ if $P \in \Omega_0$ and $s(P) = +1$ if $P \notin \Omega_0$.

Now, if we take a fixed 3D domain Ω_D that contains the free surface for all times, we can define the initial value problem for the level set function Ψ posed on Ω_D:

$$\begin{aligned} \partial_t \Psi + \mathbf{u} \cdot \nabla \Psi &= 0 \ \text{ in } \Omega_D && (16) \\ \Psi(P, 0) &= s(P)d(P) \ \text{ in } \Omega_D && (17) \end{aligned}$$

Equation (16) moves all the level set of Ψ, not just the zero level set, and in many physical applications the front velocity is just defined for points lying on the free boundary.

Therefore for this equation to be valid on the whole domain we have to extend the velocity **u** off the front [6].

Equation (9) can be directly formulated as the level set Eq. (15). For the velocity field $u(Q,t)$, the trajectory of a fluid particle at initial position Q_0 is given by the solution of

$$\begin{aligned} D_t Q &= u(R(Q_0,t),t), \\ R(Q_0,0) &= Q_0 \ . \end{aligned} \tag{18}$$

Next, let $G(P,t)$ be a functions defined on Ω_D such that for every $Q \in \Gamma_t$

$$G(Q,t) = \phi(Q,t) \ , \tag{19}$$

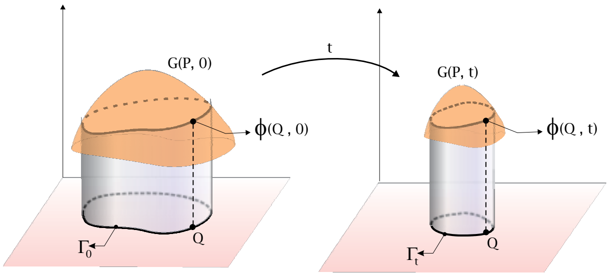

Figure 1: Extension of the velocity potential off the front

It is important to remark here that $G(P,t)$ is an auxiliary functions defined in Ω_D that can be chosen arbitrarily, the only restriction is that it equals $\phi(Q,t)$ on Γ_t. Figure 1 gives an interpretation of this property for a moving curve in 2D. Applying the chain rule in identity (19) we obtain

$$\partial_t G + \mathbf{u} \cdot \nabla G = f \tag{20}$$

which holds on Γ_t. Note that **u** and the right hand side of Eq. (20) are only defined on Γ_t, and thus, in order to solve these equations over the fixed domain Ω_D, these variables must be extended off the front.

The system of equations, written in a complete Eulerian framework, is

$$\mathbf{u} = \nabla\phi \ \text{ in } \ \Omega_t \tag{21}$$

$$\Delta\phi = 0 \ \text{ in } \ \Omega_t \tag{22}$$

$$\Psi_t + \mathbf{u}_{\text{ext}} \cdot \nabla\Psi = 0 \ \text{ in } \ \Omega_D \tag{23}$$

$$G_t + \mathbf{u}_{\text{ext}} \cdot \nabla G = f_{\text{ext}} \ \text{ in } \ \Omega_D \tag{24}$$

Here the subscript “ext” denotes the extension of f and **u** onto Ω_D.

The numerical approximation of this coupled system of PDEs Eqs.(21)-(24) can be described in two basic steps. The time derivatives in the level set equations are approximated using a standar first order backward Euler scheme and the space derivatives a first order upwind scheme. At each time step, Eqn. (22) is solved using its Boundary integral formulation and a Boundary linear element approximation is used. The complete details of the numerical approximation can be found in [7], [9], [11].

4 EXAMPLES OF POTENTIAL FLOW MODELS WITH MOVING BOUNDARIES

4.1 The wave breaking problem

The coupled level set/extension potential equations for breaking waves is set in two dimensions. Let Ω_t be the $2D$ fluid domain in the vertical plane (x, z) at time t, with z the vertical upward direction (and $z = 0$ at the undisturbed free surface), and Γ_t the free boundary at time t (see Figure 2).

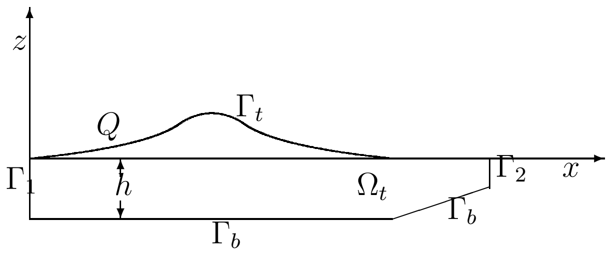

Figure 2: The domain

For this case, surface tension forces will not be considered and thus the expression of f in Eqn. (24) is

$$f = \frac{1}{2}\mathbf{u}^2 - gz.$$

Here we have to add the boundary condition on the rest of the fluid boundary, $\phi_n = 0$ on $\Gamma_b \cup \Gamma_1 \cup \Gamma_2$.

A complete numerical convergence study for the wave breaking problem can be found in [7], [8], where it has been also studied the influence of the beach bottom profile on the wave breaking characteristics. Here, in Fig. 3 we just show the case of a solitary wave with initial heigh $H_0 = 0.6$ shoaling, turning and breaking over a mild constant slope of $1 : 22$.

4.2 The Rayleigh Taylor instability

A significant challenge in the numerical solution of free boundary problems is when the domain undergoes topological changes. This is the case of the Rayleigh-Taylor instability of a fluid column of length L, in which an small initial perturbation of wave number $k = \frac{2\pi}{L}$ will lead to the fluid overturning, pinch-off and subsequent cascade of drop formation. To model this problem we have used the axisymmetric version of the coupled level

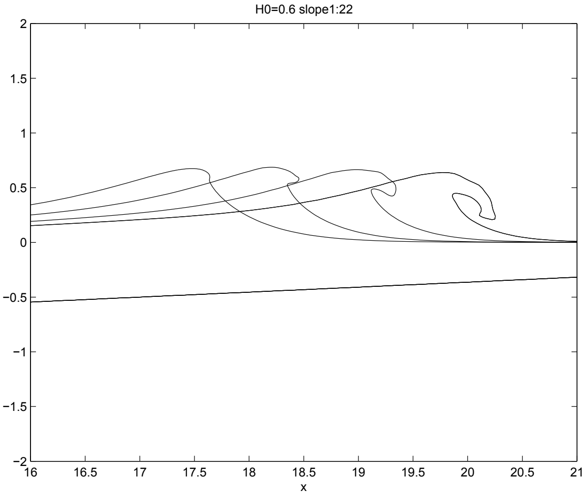

Figure 3: Wave shape at various times for a beach slope of 1 : 22

set/extension potential equations and the cylinder geometry in the (r, z) plane is depicted in Fig. 4.

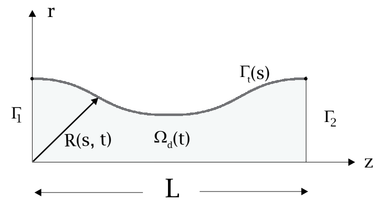

Figure 4: Cylinder geometry in the $r - z$ plane.

Here, surface tension forces have to be considered, being the dominant forces in this scenario. The pressure jump across the free bounday is $p = p_a + \gamma\kappa$, where γ is the surface tension coeficient and κ is twice the mean curvature of the moving surface. As the effects of gravity are neglected, the expression of f in Eqn. (24) is

$$f = \frac{1}{2}\mathbf{u}^2 - \frac{\gamma}{\rho}\kappa.$$

Periodic boundary condition on the lateral walls of the cylinder are imposed.

An extensive numerical study and validation of the collapse of a fluid column is presented in [9]. In Fig. 5 we show the fluid column overturning, just prior to pinch-off. After separation the satellite drop undergoes its own instability and it pinches-off in its middle point. This originates capillary waves propagating on the satellite surface, which lead to a cascade of drop formation, including fast separations and reconnections. Comparisson with Laboratory experiments and self similar scaling laws can also be found in [9].

4.3 Drop distortion under the action of an electrical field

For this problem we consider a perfectly conducting inviscid fluid droplet of density ρ sourrounded by a dielectric gas of permittivity ϵ and exposed to the action of an uniform electric field at infinity. Here we have to couple the potential fluid equations that govern the interior drop dynamics with the electrostatic assuptions for the exterior gas. As the ambient medium is considered uniform and uncharged, the electric field is the gradient of an electric potential W,

$$\begin{aligned} \mathbf{E} &= -\nabla W \quad \text{in } \Omega_2(t) &(25)\\ \Delta W &= 0 \qquad \text{in } \Omega_2(t) &(26)\\ W &= W_0(t) \quad \text{on } \Gamma_t &(27)\\ W &= -E_\infty z \quad \text{at infinity} &(28)\end{aligned}$$

The electric stresses at the free surface elongate the drop against the restoring effect of the surface tension and the pressure jump across the free surface Γ_t is given by

$$p = p_a + \gamma\kappa - \frac{\epsilon}{2}E_n^2, \tag{29}$$

where $E_n = -\nabla W \cdot \mathbf{n}$, $\mathbf{n}$ the unit normal vector pointing from the interior to the exterior domain. In this case the right hand side expresion for Eqn. (24) is

$$f = \frac{1}{2}\mathbf{u}^2 - \frac{\gamma}{\rho}\kappa - \frac{\epsilon}{2\rho}E_n^2.$$

The complete model can be written in its non-dimensional form, where the only parameter left is the non-dimensional electric field intensity. Theoretical and experimental studies show that there exists a critical value $E_c \approx 0.3$ such that for $E_\infty < 0.3$ the drop oscillates with known frequency, while for $E_\infty > 0.3$ the drop is distorted in the direction of the electric field. A cone singularity (the taylor cone) appears from which thin jets are ejected. In Fig. 6 we depict the drop profiles at various times: the drop elongates and finally pinches-off and jet discharge occurs. Laboratory photographs, kindly provided by Grimm and Beauchamp, are shown on the left for two different electric field intensities; on the right the corresponding numerical profiles are also shown. A complete study of electrostatically driven jets fron non-viscous droplets will be presented elsewhere [12].

5 CONCLUSIONS

- The Eulerian formulation in 3 dimensions of the fully nonlinear potential flow model has been derived using the Level Set technique, which automatically includes topological changes of the free boundary. The numerical approximation of the coupled Level Set-Boundary Integral equations uses very simple first order numerical schemes, which are proved to be enough to capture complex non viscous fluid dynamics.

- Very interesting phenomenons, such as wave breaking, the collapse and pinch-off of a fluid column and the distortion of droplets under the action of an electric field, are successfully simulated using this novel algorithm. We briefly show some results and address to the proper references.

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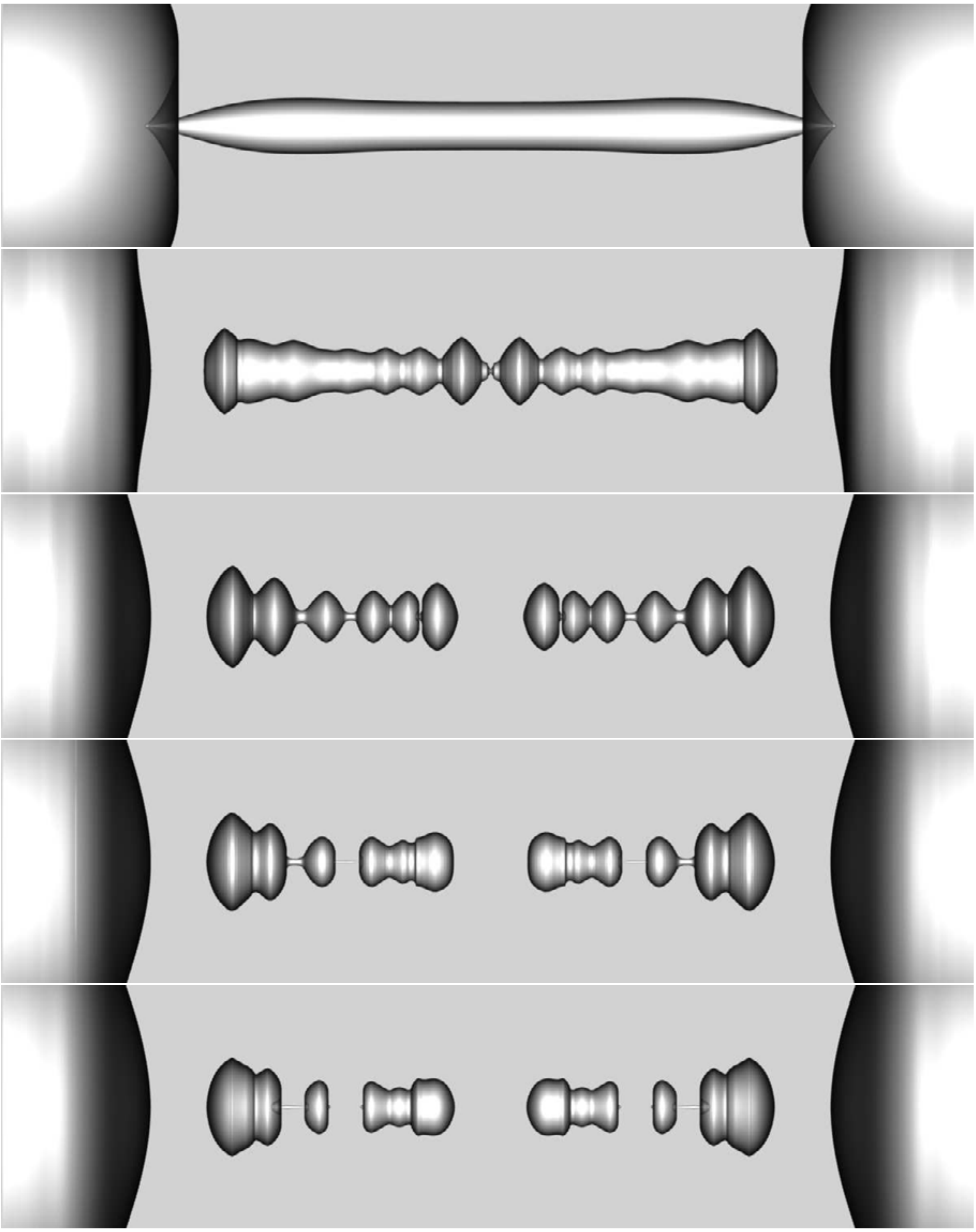

Figure 5: Fluid column overturning and pinching followed by a cascade of drop formation, top to bottom

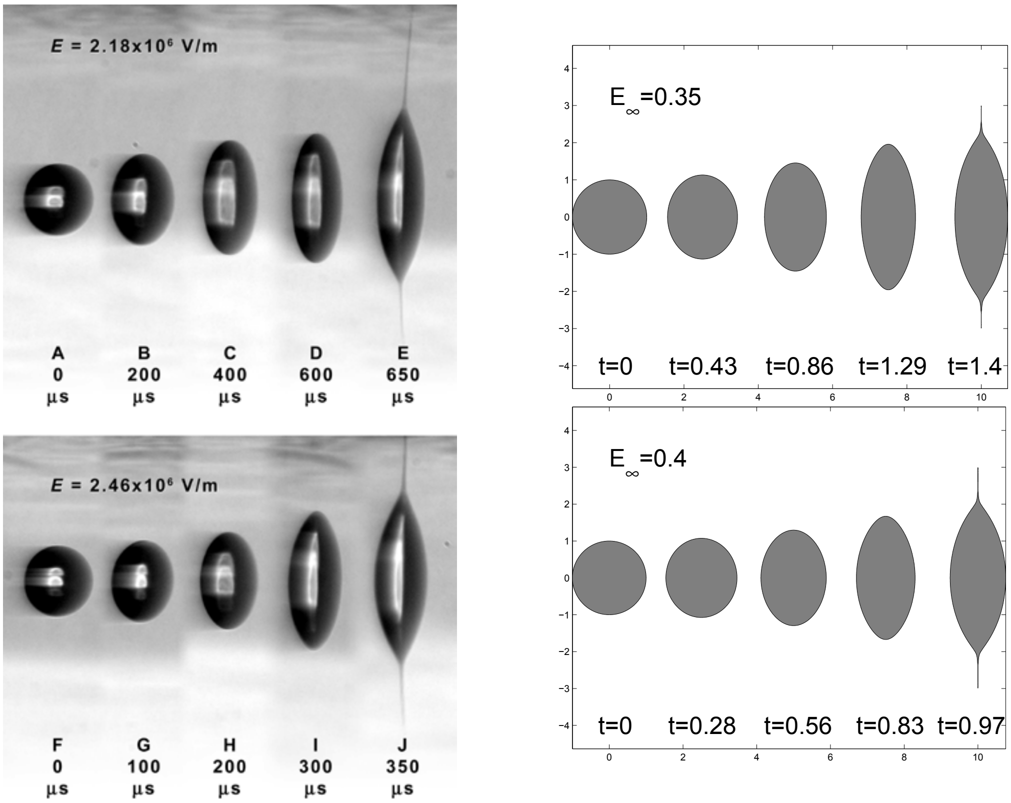

Figure 6: Laboratory photograph left; computational profiles right at indicated times